The Crystalline Structure of Herderite, Datolite and Gadolinite

of isostructure-gadolinite. Its formula is obtained from the datolinite-formula CaBSiO OH by replacement of the 5-charge-pair CaB by YBe and introduction into the inversion-centers of the cell (cf. figure 3 in reference 5) of 2 additional Fe with a simultaneous replacement of 4 OH by 4 O. This leads to the formula FeY 2 -Be₂Si₂O₁₀ in the case of 2 such "molecules" in the cell. An analysis similar to the above-mentioned ones was carried out for gadolinite. 30 of very strong inequalities in this case had determined 40 signs of supporting group. The second projection of the electron-density is shown on figure 3, the coordinates following from it in the fourth column of table 1. The quality of the radiogram was worse by the inclination to metamictic disintegration of gadolinite, and due to the indetermination of the atom-factor of \tilde{Y} (Z = 39) whose major part is on the one hand replaced by Er (Z = 68) and on the other hand by Ca (Z = 20). It is easy to realize that the atom-coordinates of gadolinite are closer to those of herderite than to those of datolite, as a Be-atom with a radius much larger than that possessed by B in datolite is part of the two first minerals. There are 3 figures, 1 table, and 6 references,

Card 3/4

The Crystalline Structure of Herderite, Datolite and Gadolinite

SUBMITTED: April 4, 1957

Card 4/4

SHUBNIKOV, Aleksey Vasileyevich, akademik; BRLOV, N.V., akademik, otvetstvennyy red.

[Crystals in science and engineering] Kristally v nauke i tekhnike. Izd.2., dop. Moskva, Izd-vo Akad. nauk SSSR, 1958. 53 p.
(Crystals) (MIRA 11:7)

BELOV, N.V.

3(8) h_3 Phase I book exploitation sov/1310

- Soveshchaniye po eksperimental'noy i tekhnicheskoy mineralogii i petrografii, 5th Leningrad, 1956.
 - Trudy... (Transactions of the Fifth Conference on Experimental and Applied Mineralogy and Petrography) Moscow, Izd-vo AN SSSR, 1958. 516 p. 1,800 copies printed.
 - Sponsoring Agency: Akademiya nauk SSSR. Institut geologii rudnykh mestorozhdeniy, petrografii, mineralogii i geokhimii, and Akademiya nauk SSSR. Institut khimii silikatov.
 - Resp. Ed.: Tsvetkov, A.I.; Ed. of Publishing House: Ivanov, B.V.; Tech. Ed.: Kiseleva, A.A.
 - PURPOSE: This book is intended for scientists and students of mineralogy and petrography.
 - COVERAGE: The present collection of articles are reprints of reports presented at the Fifth Conference on Experimental and Applied Mineralogy and Petrography, held in Leningrad on March 26-31, 1956. The

Card 1/11

Transactions of the Fifth Conference (Cont.)

SOV/1310

purpose of the Conference was to exchange information and coordinate the activities in the fields of experimental and applied mineralogy and petrography, and to stress the increasing complexity of practical problems. The Conference was sponsored by the Academy of Sciences of the USSR and organized by its Institute of Ore Deposits, Geology, Petrography, Mineralogy and Geochemistry of the Division of Geological-Geographical Sciences, and the Institute of Silicate Chemistry of the Division of Chemical Sciences. During the Conference special tribute was paid to Academician D.S. Belyankin, (died 1952), founder of applied petrography in the USSR and organizer of the first four conferences and Academician A.N. Zavaritskiy, (died 1953), outstanding petrographer and mineralogist. Of the 76 reports presented, 53 are reprinted in the present volume. Each article is accompanied by diagrams, tables, and bibliographic references.

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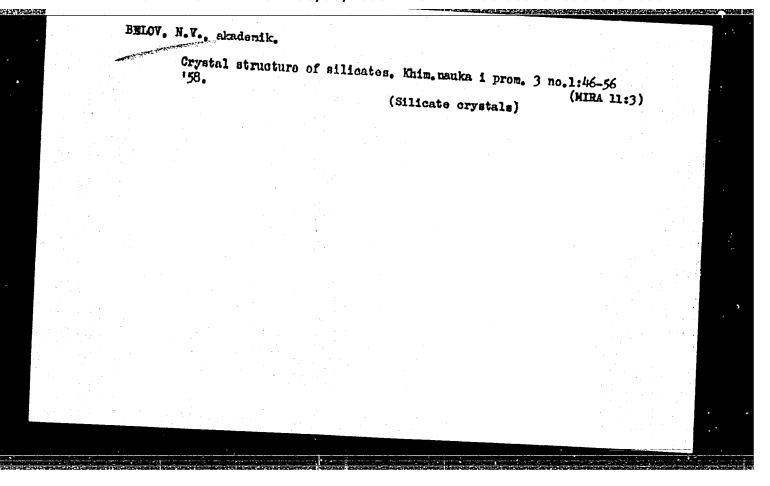
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AUTHOR:

Belov, N. V., Member, AS USSR

30-58-3-12/45

Vaynshteyn, B. K., Doctor of Physical and

Mathematical Sciences

TITLE:

The Congress of Crystallographers Held at Montreal

(Kongress kristallografov v Monreale)

PERIODICAL:

Vestnik Akademii Nauk SSSR, 1958,

Nr 3.

pp. 64-67 (USSR)

ABSTRACT:

The fourth congress took place in the summer of last year and was attended by more than 700 scientists from 21 countries. The Soviet delegation consisted of N. V. Belov, L. M. Belyayev,

G. B. Bokiy, Ye. G. Bronnikova, B. K. Vlynshteyn, G. S. Zhdanov, V. I. Iveronova, A. I. Kitaygorodskiy, Z. G. Pinsker

and S. I. Shchetimin. They had a special number of the

periodical "Crystallography" taken with them, which contained all reports delivered by the delegation on this congress, as well as a collection of scientific investigations The Growth of Growth of Crystals". The work of this congress was carried out by 18 sections. In the plenary sessions lectures were delivered on topical problems of modern crystallography.

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The Congress of Crystallographers Held at Montreal

30-58-3-12/45

On the last two days special symposia on electronography and on the physical research methods of crystallography were held. Great importance was attached to consultations held outside the official sessions on various scientific problems. A large group of reports dealt with the theory, the method, and the new results obtained by investigations on the atomic structure of crystals. In the section "Progress in Structural Determination", A. I. Kitaygorodskiy among other things, dealt with the correlation theory among structural factors. Much attention was paid to electronic computers. Also new types of apparatus were on show in special exhibitions of this congress. N. V. Belov reported on new silicate structures. The authors regretted the fact that, in the field of structural determination, mainly only such structures were precisely dealt with as are already known. A report on general problems of crystal chemistry was delivered by G. Shdanov. The report by G. B. Bokiy and G. A. Kukina dealt upon the crystal chemistry of the complex compounds of bivalent platinums. A. I. Kitaygoroskiy spoke about several results achieved in the

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The Congress of Crystallographers Held at Montreal

30-58-3-12/45

investigation of organic structures at the Institute for Organoelementary Compounds of the AS USSR. Z. G. Pinsker spoke about the results obtained by electronographic investigations of some carbides and nitrites. Radiographic investigations of displacements were dealt with by V. I. Iveronova. L. M. Belyayev delivered a report on the investigation of a distribution of activators in halide-crystals of alkaline metals. Ye. G. Bronnikovs gave a survey of the methods of breeding piezo-electric crystals in the USSR. On a plenary session the Soviet delegation showed the film. "The crystallization of two-teased diphenylamine (dvulistnikov difenilamine). In the section dealing with the symmetry theory N. V. Belov, reported on the 1651 group of the spatial black- and white, as well as on groups of colored symmetry. In a symposium Z. G. Pinsker and B. K. Vaynshteyn delivered a lecture on problems of structural electronography and its development in the USSR. B. K. Vaynshteyn gave a report on electron dispersion by means of crystalline polydispersion preparations. Parallel to the congress a full session of the

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The Congress of Crystallographers Held at Montreal

30-58-3-12/45

Society of Crystallographers was held, on which occasion new elections were finally carried out as the result of which N. V. Belov was elected vice-president for 6 years and other Soviet scientists were elected members of various commissions. The Soviet delegation was able to visit scientific research laboratories of the universities of Montreal and in the vicinity of this town, as well as the National Research Center in Ottawa. They were able to convince themselves of the high level of these institutions. The congress showed that crystallography is developing according to plan.

Card 4/4

AUTHOR:

Belov. N.V.

SOV/70-3-1-16/26

TITIE:

On the Law of the (X-ray) Extinctions in Quartz

(O kvartsevom zakone pogasaniy)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 1, pp 89-90 (USSR)

ABSTRACT: In B. Ya. Pines' book, "Lectures on X-ray Structure Analysis", second edition, Khar'kov, 1957, the law h + k + l = 3n is found for the reflections from the rhombohedral cell of This is not found in the International Tables or other standard handbooks. This is likely to cause confusion and is an archaism. It arises from an old classical tradition of using a triply primitive rhombohedral unit cell (extra lattice points at 1/3, 1/3, 1/3 and 2/3, 2/3, 2/3) which corresponds with the observed external

It is the rhombohedral cell in terms of which a

hexagonal primitive cell can be expressed.

The error that four indices are desirable for the expression of co-ordinates and axes in the hexagonal system is also found. Belov demonstrates that h + k + i = 0 and that the fourth index is redundant but desirable for faces but meaningless and confusing for axes and co-ordinates.

CIA-RDP86-00513R000204510007-2 "APPROVED FOR RELEASE: 06/06/2000

On the Law of the (X-ray) Extinctions in Quartz

There are 2 figures and 5 Soviet references

Institut kristallografii AN SSSR (Institute of Crystallography of the Ac.Sc.USSR) ASSOCIATION:

SUBMITTED: December 13, 1957

Card 2/2

SOV/70-3-1-17/26 AUTHORS: Borisov, S.V., Pavlov, P.V. and Belov, N.V.

TITIE:

A Graphical Method for Solving the Fundamental Harker-Kasper Inequalities (Graficheskiy metod resheniya

osnovnykh neravenstv Kharkera-Kaspera)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 1, pp 90-92 (USSR)

ABSTRACT: The most powerful inequality relating the absolute unitary structure amplitudes is:

 $(\mathbf{U}_{\mathrm{H}} \pm \mathbf{U}_{\mathrm{K}})^{2} \leq (1 \pm \mathbf{U}_{\mathrm{H+K}})(1 \pm \mathbf{U}_{\mathrm{H-K}})$

This leads to a relationship between the signs of $S_{H+K} = S_{H} \cdot S_{K}$ and $S_{H-K} = S_{H} \cdot S_{K}$. The examination of all quartets of reflections is a long process and can be facilitated by suitable graphs. If $(U_H \pm U_K)$ is denoted by $\sum_{k=1}^{\infty}$ and $(1 \pm U_{H+K})$ and $(1 \pm U_{H-K}) > by x$ and y, respectively, then the inequality is Σ^2 which takes the form of hyperbolae for the case of equivalence. Lines of constant Σ are drawn out on two graphs (each with U_{H-K} as abscissae and U_{H+K} as

Cardl/3 ordinates) one with values of Σ greater than 1 and

A Graphical Method for Solving the Fundamental Harker-Kasper Inequalities

the other with values less than 1. The graphs are then divided into four regions: a) where $S_{H-K} = S_H \cdot S_K$ obtains; b) where $S_{H+K} = S_H \cdot S_K$ obtains; c) where neither obtains and ab) where both are true. These can be overlaid with weighted reciprocal nets. It can be seen that the most effective inequalities will be obtained when three of the amplitudes selected are large and the fourth small. For values of Σ near to 1 the inequalities will also be effective, for a pair U_{H+K} and U_{H-K} of the order of 0.15 to 0.20. There are 3 figures and 7 references, 5 of which are Soviet and 2 English.

Card 2/3

A Graphical Method for Solving the Fundamental Harker-Kasper Inequalities

ASSOCIATION:

Institut kristallografii AN SSSR (Institute of Crystallography of the Ac.Sc.USSR)

SUBMITTED:

November 25, 1957

Card 3/3

AUTHOR: Belov, N.V.

70-3-2-15/26

THE REPORT OF THE PROPERTY OF

TITLE:

The Facial Morphology of Crystals in the Light of Their Fine Structures (Grannaya morfologiya kristallov v svete ikh

tonkoy struktury)

PERIODICAL:

Kristallografiya, 1958, Vol 3, Nr 2, pp 225 - 227 (USSR)

ABSTRACT: Criticisms are made of statements in a new book "Kristally mineralov" by I.I. Shafranovskiy (Leningrad, 1957). Tables are given on pp 90 - 106 of the symmetries of the general and special faces of crystals belonging to the 230 space groups. Satisfactory agreement is found with observations on 8 cubic minerals but garnet appears to be an exception. In this case, a cube and not a rhombic dodedahedron has the most symmetrical faces but garnet (space group Oh = Ia3d) crystallises in the dodecahedral form 110. The whole argument in this section is shown to be fallacious and certain additional errors of fact are pointed out. There are 2 figures and 6 references, 4 of which are Soviet and 2 French.

ASSOCIATION:

Institut kristallografii AN SSSR (Institute of

Crystallography, Ac.Sc. USSR)

SUBMITTED: Card 1/1

February 7, 1958

AUTHOR: Belov, N.V.

70-3-2-25/26

On ways or founding a Correct Soviet Course in Crystallography (O putyakh k sozdaniyu polnotsennogo sovetskogo kursa kristallografii)

PERIODICAL:

Kristallografiya, 1958, Vol 3, Nr 2, pp 246 - 249

ABSTRACT:

Mrrors in Soviet Textbooks, published since 1950, when dealing with questions of symmetry are quoted and examined. References to the books criticised are not given. Foreign books are not exempt from the failings castigated.

ASSOCIATION:

Institut kristallografii AN SSSR

(Institute of Crystallography, Ac.Sc. USSR)

SUBMITTED:

February 7, 1958

Card 1/1

AUTHORS: 70-3-2-26/26

Belev, N. V., Belyayev, L.M., Bokiy, G.B., Bronnikova, Ye.G., Vaynshteyn, B.K., Zhdanov, G.S., Iveronova, V.I., Kitaygorod-skiy, A.I. and Pinsker, Z.G.

TITLE:

The Fourth International Congress of Crystallography (IV mezhdunarodnyy kongress kristallografov) (Montreal, July 10-19, 1957)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 2, pp 250 - 260

ABSTRACT: Outline of the scientific proceedings of the

conference.

. Card 1/1

USCOMM-DC-60577

Borisov, S.V., Golovachev, V.P. and Relov AUTHORS:

TITLE:

On the Arbitrary Allocation of Signs in Direct Methods of Determining Crystal Structures (O proizvol'no zadavayemykh znakakh pri pryamykh sposobakh rasshifrovki kristallich-

eskikh struktur)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 3, pp 269 - 276

ABSTRACT: The limiting conditions on the arbitrarily allocated signs of three-structure amplitudes which are connected with the use of the direct methods of analysis are worked out and tabulated for all symmetries except inversion. The equivalent groups of centres of symmetry are listed for the seven crystal systems with lattices of the P, C, I and F types and under the headings of the Bravais lattices, the equivalent centres for the tabulated forms of the structure factors, the groupings of the different classes of reflections, the number of arbitrarily assignable signs and the types of reflections for which it is not permissible to allocate signs arbitrarily are tabulated. The same types of information are also given for the plane groups. Such data is not available elsewhere in organised form. There are 6 figures, 3 tables and 8 references, Cardl/2 l of which is Soviet and 7 English.

CIA-RDP86-00513R000204510007-2 "APPROVED FOR RELEASE: 06/06/2000

On the Arbitrary Allocation of Signs in Direct Methods of Determining Crystal Structures 70-3-3-2/36

ASSOCIATION:

Institut kristallografii AN SSSR (Institute of Crystallography, Ac.Sc. USSR)

SUBMITTED:

March 14, 1958.

Card 2/2

AUTHORS:

Simonov, V,I. and Belov, N.V.

SOV/70-3-4-5/26

TITLE:

A Determination of the Structure of Ambligonite by the Method of Minimalisation (Opredeleniye struktury

ambligonita metodom minimalizatsii)

PERIODICAL:

Kristallografiya, 1958, Vol 3, Nr 4, pp 428-437 (USSR)

ABSTRACT:

A full determination of the structure of crystals of LialPOut has been made by a superposition process. resolving power of the function used has been estimated and the crystal-chemical properties of lithium have been elucidated. The triclinic cell of a natural specimen with small sodium content was found to have the dimensions a = 5.06, b = 5.16, c = 7.08 A; $\alpha = 109^{\circ}52'$, $\beta = 107^{\circ}30'$, $\gamma = 97^{\circ}54'$. Previous authors have chosen different axes but their measurements agree with the above. Three Weissenberg photographs were taken of equatorial layer lines with Mo radiation and intensities were estimated visually, 218 Ok1, 190 hol and 167 hk0 reflections were recorded. The statistics of the hOl zone showed it to be centred and implied that the space group

was $Pl = C_1^1$ Z = 2. The Patterson projections p(x,z)

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A Determination of the Structure of Ambligonite by the Method of

and p(y,z) were calculated. If \underline{r}_0 represents a Patterson peak with a radius vector \underline{r}_0 , then several superposition functions are available, in particular:

$$\sum = P(\underline{r} - 1/2 \underline{r}_0) + P(\underline{r} + 1/2 \underline{r}_0)$$

$$\prod = P(\underline{r} - 1/2 \underline{r}_0) \cdot P(\underline{r} + 1/2 \underline{r}_0)$$

$$M = \min \left\{ P(\underline{r} - 1/2 \underline{r}_0), P(\underline{r} + 1/2 \underline{r}_0) \right\}$$

$$I = \sum_{z_0} \left| P(\underline{r} - 1/2 \underline{r}_0), \quad P(\underline{r} + 1/2 \underline{r}_0) \right|$$

$$I = \sum_{z_0} \left| P(\underline{r} - 1/2 \underline{r}_0) - P(\underline{r} + 1/2 \underline{r}_0) \right|$$

and M = 1/2 I.

The P-Al and P-P peaks were identifiable in the Patterson projections and, as the M function was shown to be the most powerful, it was calculated for the x,z and y,z projections with the vectors P-P and Al-Al and enabled oxygen positions to be found. The corresponding

Card 2/4

A Determination of the Structure of Ambligonite by the Method of Minimalisation

structure factors were calculated and electron density projections constructed with very satisfactory agreement. It was concluded that the Li atoms were distributed statistically between two positions, final R values (incl. zero reflections) of about 15% being obtained. The final co-ordinates were: (x,y,z) Al_I (0,0,0); Al_{II} (0.50, 0.50, 0.50); P (0.565, 0.883, 0.238); O_I (0.646, 0.680, 0.3485); O_{II} (0.659, 0.194, 0.402); O_{III} (0.724, 0.836, 0.0805); O_{IV} (0.234, 0.795, 0.1115); (F,OH) (0.143, 0.319, 0.267); 1/2 Li_I (0.92, 0.575, 0.18); 1/2 Li_{II} (0.995, 0.65, 0.25). The accuracy is estimated at P ± 0.002 A, O ± 0.005 A, 1/2 Li ± 0.05 A. Diagrams are given of the ways in which the P tetrahedra and the Al octahedra link up and a calculation of the way in which

Card 3/4

Belov, N.V., Belova, Ye.N. and Tarkhova, T.N. AUTHORS: TITIE:

Further on the Colour Symmetry Groups (Yeshche o

gruppakh tsvetnoy simmetrii)

PERIODICAL: Kristallogafiya, 1958, Vol 3, Nr 5, pp 618-620 (USSR)

ABSTRACT: Diagrams of the 15-colour symmetry groups which were given in Kristallografiya, 1957, Vol 2, p 21 can be improved slightly. The designation of the group I 41

is altered to I $4_1(4_3)$ and its relationship to the

packing of squares, each of symmetry P 41, is illustrated.

New diagrams are given showing the symmetries of the groups I 41md and Fdd2 better than those published

previously. There are 18 figures and 5 Soviet references.

ASSOCIATION:

Institut kristallografii AN SSSR (Institute of Crystallography of the Ac.Sc.USSR) SUBMITTED:

July 11, 1958

Card 1/1

AUTHORS: SOV/70-3-5-22/24

Donnay, G., Belov, N.V., Neronova, N.N. and Smirnova, T.S. TITIE:

On the Shubnikov Groups (O Shubnikovskikh gruppakh) (Letters to the Editor)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 5, pp 635-636 (USSR)

Letter from the first author. Baltimore, USA, April 12,

It is suggested that in the deduction of the 36 Pg groups of the Subnikov (black and white) groups 12 groups are not distinct but me only repetitions in different orientations of others. 12 other groups are thought

to have been omitted.

Derivations of the groups 387 (Paccm) and 388 (Pabmb) are taken as examples. It is found that Pabmb must be replaced by Pamaa . The co-ordinates of the black and white equivalent points in the 3 groups are listed. All co-ordinates of Pabmb can be transformed into those of

Paccm by the following matrix: the co-ordinates of the black and white points are exchanged. No matrix will

Card 1/3

On the Shubnikov Groups

SOV/70-3-5-22/24

transform co-ordinates in Pama into those in Paccm. The simple rule is that if the x- co-ordinates are identical for two settings connected by a transformation matrix, then the two Pa-symbols will correspond to different settings (aspects) of the same Shubnikov group. The groups following are therefore doublets (numbers as in Trudy Inst. Kristallog., 1955, Vol 11, p 33): 372, 371; 374, 373; 377, 375; 380,378; 385, 384; 388, 387; 390, 389; 392, 391; 394, 393; 395, 396; 400, 399; 402, 403.

The following groups should be added Pamaa, Panch, Pahm, Pabaa, Pamch, Panaa, Pahm, Paman, Paman.

Reply from the other authors, Moscow, July 4, 1958: These mistakes have already been acknowledged and corrected in Kristallografiya, 1957, Vol 2, Nr 3, pp 315-25.

Card 2/3

On the Shubnikov Groups

SOV/70-3-5-22/24

Canonical forms of the 12 additional groups listed above are given, together with the group numbers and equivalent groups. All are preferred in the setting P_a as above.

There are 2 Soviet references.

July 11, 1958 SUBMITTED:

Card 3/3

AUTHOR:

Belov, N.V.

SOV/70-3-6-25/25

TITIE:

Plan for a University Course in Space Groups (Proyekt vuzovskogo kursa fedorovskikh grupp)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 6, pp 765-772 (USSR)

ABSTRACT: Outline of a system of teaching symmetry and, in particular, the 230 space groups in logical way. There are 5 references, 4 of which are Soviet and

ASSOCIATION:

Institut kristallografii AN SSSR

(Institute of Crystallography of the Ac.Sc.USSR)

SUBMITTED:

September 8, 1958

Card 1/1

20-119-2-45/60

· AUTHORS:

Simonov, V. I., Belov, N. V., Member, Academy of Sciences,

TITLE:

The Crystalline Structure of Amblygonite (Kristallicheskaya

struktura ambligonita)

PERIODICAL:

Doklady Akademii Nauk SSSR, 1958, Vol. 119, Nr 2,

PP# 354 - 356 (USSR)

ABSTRACT:

Initially the amblygonite LiAlPO4(F,OH) is charaterized in

detail (Reference 2). The amplitude statistics Fhol have con-

firmed the presence of a center of symmetry in the amblygonite. Paterson's projections p(x, z) and p(y,z) made the

regularities of the centrosymmetric crystals be seen (Reference 4) which made possible the elimination of the vector-branches, which correspond to the distances between the atoms; the latter

are connected to the center of symmetry. Moreover the mini-

Card 1/4

mizing (References 5,6) could be carried out according to the projections. The approximated values of the coordinates of all

20-119-2-46/60

The Crystalline Structure of Amblygonite

atoms apart from Li could be determined from $M_4(x,z)$ and $M_2(y,z)$ (Reference 7). The precision of the structure was carried out according to the projections of the electron density $\sigma(x,y)$, $\sigma(z,z)$, $\sigma(y,z)$ without taking Li into consideration. The precision process was continued according to the latter with the same signs according to which the latter projections were built up, until the converted signs of all amplitudes F and F okl (for F or F or

Card 2/4

The Crystalline Structure of Amblygonite

20-119-2-46/60

conclusion has been confirmed by the calculated coefficients of the authencity R for different possible positions of Li. The assumed coordinates of the base atoms of the amblygonite - 2 kinds of Al without parameter (in centers of symmetry) and 7 other atoms in common positions with 24 parameters (li has statistically 2 positions) - are collated in table 1. The common anions (F, OH) unite the Al-octahedra in chains parallel to the line b1. The bands of the alternating P- tetrahedra and Li-polyhedra extend in the same direction. The tetrahedron-octahedron-bands are combined in lattices which are at right angles to the direction c1. Figure 3 shows the projection of a lattice with Al and P, but instead of Li-polyhedra positions are given which are taken by Li with a probability of 1/2. Moreover interatomic distances in the amblygonite are given. The assumption of a structural relationship between amblygonite and herderite (Reference 9) is not confirmed, as in the structure of the amblygonite, lattices exclusively consisting of tetrahedra or octahedra are lacking. There is, however, a similarity of the chains in the amblygonite with those in sphene CaTiSiO5. There are 3 figures,

Card 3/4

The Crystalline Structure of Amblygonite

20-119-2-46/60

1 table and 11 references, 5 of which are Soviet.

SUBMITTED:

December 30, 1957

Card 4/4

AUTHORS:

Mamedov, Kh. S. Relov, N. V., Member, Academy of Sciences, USSR

SOV/20-121-4-40/54

TITLE:

The Crystalline Structure of Micaceous Calcium Hydrosilicates: Okenite, Nekoite, Truscottite, Gyrolite (Kristallicheskaya struktura slyudopodobnykh Ca-gidrosilikatov: okenita, nekoita, truskottita, girolita) A New Silicon-Oxygen Radical (Si6015)

(Novyy kremnekislorodnyy radikal (Si6015) 00)

PERIODICAL:

Doklady Akademii nauk SSSR, 1958, Vol. 121, Nr 4,

pp. 720 - 723 (USSR)

ABSTRACT:

It is well known that from silicon-oxygen chains of pyroxene (SiO3) amphibole bands are formed as a consequence of

their duplication (with respect to the plane of symmetry). They are composed of members of 6 subdivisions each and may be polymerized to 2-dimensional lattices (Si205) e. These

lattices have only 6-membered loops which are a characteristic feature of the very comprehensive class of pseudo-hexagonal strata of minerals: Mica, loams, chlorites. The pyroxenoid chains $(Si0_3)_{\infty}$ with a different geometry which the author

Card 1/4

The Crystalline Structure of Micaceous Calcium Hydro- SOV/20-121-4-40/54 silicates: Okenite, Nekoite, Truscottite, Gyrolite. A New Silicon-Oxygen

discovered in wollastonite (Ref 1) (3 Si-tetrahedrons in the member compared with only two in pyroxenes) yield in bands with a different formula (Si6017) as a result of duplication, and with 8-membered chains (xonolite bands (Ref 2)) which polymerize to lattices with a very much feature of wollastonite xonolite and of related Ca-minerals are infinite columns of Ca-octahedrons which are added in such a way that the 0 - 0-edge of each of them is directly continued by the edge of the next (Fig 1 b). Such an edge is much longer than that of a Si-tetrahedron but is less than its double height. Thanks to the inclination of the tetrahedrons on one edge of a Ca-octahedron a pair of Si-tetrahedrons is attached whereas to a following Ca-tetrahedron corresponds an edge of a Si-tetrahedron + "saved component" which was formed by the previous Si-tetrahedron pair thanks to the inclination. Since the edges of both Ca-tetrahedrons

Card 2/4

The Crystalline Structure of Micaceous Calcium Hydro- SOV/20-121-4-40/54 silicates: Okenite, Nekoite, Truscottite, Gyrolite. A New Silicon-Oxygen

are equal this holds also true for the two modifications of the conjugate chain of Si-tetrahedrons. Thus such a combination of the near xonolyte bands is possible as it is shown on figure 1 v. The conjugating element of symmetry is the slip plane which is most natural in microcrystallography. In the chain an exchange takes place between 8-membered rings with the double number of 5-membered rings. When heated up to 800° okenite decomposes to wollastonite and a nonorientated crystobalite which process is accompanied by a loss of H20. The formation of an oriented wollastonite due to dehydration obviously points to the fact that the decomposing radical is a condensate of the wollastonite chain (Ref 6). The final crystallochemical okenite formula is the following: 3/Ca₃Si₆O₁₅.2H₂O.4H₂O/. Also the thermogram with 2 clear endothermal maxima corresponds to the separation of water into constitution- and zeolite water. There are 4 figures, 1 table, and 10 references, 5 of which are Soviet.

Card 3/4

The Crystalline Structure of Micaceous Calcium Hydrosilicates: Okenite, Nekoite, Truscottite, Gyrolite. A New Silicon-Oxygen SOV/20-121-4-40/54 Radical (Si₆0₁₅)∞

ASSOCIATION: Institut khimii Akademii nauk AzerbSSR (Chemical Institute, AS Azerbaydzhan SSSR) Institut kristallografii Akademii nauk SSSR (Institute of Crystallography, AS USSR)

SUBMITTED:

April 29, 1958

Card 4/4

AUTHORS:

Mamedov, Kh. S., Belov, N. V.,

SOV/20-121-5-37/50

Member, Academy of Sciences, USSR

TITLE:

Crystalline Structure of Foshagite Ca₈[Si₆O₁₇](OH)₆

(Kristallicheskaya struktura foshagita Ca_R Si₆O₁₇ (ON)₆)

PERIODICAL:

Doklady Akademii nauk SSSR, 1958, Vol. 121, Nr 5,

pp. 901-903 (USSR)

ABSTRACT:

The authors introductorily discuss the previous versions of the formulae of this mineral belonging to the fibrous hydrated wollastonites (Refs 1 - 5). It is a typical fibrillar mineral. Besides powder diagrams, also X-ray diagrams of the rotation about the fiber-axis can be obtained from it. The

corresponding lattice period amounts to 7,35 Å, the pseudo-

semiperiod 3,68 Å, however, is distinctly marked which is characteristic of several Ca-silicates (Refs 1,2). Foshagite is similar to xonontlite with respect to the temperature at which the main quantity of water is removed (650 to 750° according to reference 5). Similar to the Ca-minerals mentioned

Card 1/3

Crystalline Structure of Foshagite Ca₈ [Si₆O₁₇](OH)₆

SOV/20-121-5-37/50

above, foshagite, heated up to 8000, after dehydration transforms into β -wollastonite, the fibers of which are orientated parallel to those of the initial foshagite. The above mentioned period and semiperiod are equal to the two latter and to the previously mentioned minerals. The parameters of the monoclinic cell of foshagite (Ref 5) are given. The basic cleavage - at (001) - and a less marked one - at (100) were determined by means of an electron microscope (Ref 5). The authors discuss the views developed by Gard and Taylor (Ref 5). Contrary to this reference, the authors have given a practically more convenient description of \$A-wollastonite (Ref 7); there are two superfluous Ca(OH), in it, compared with wollastonite. The authors subsequently denote foshagite as a monontlite enriched with lime; $\operatorname{Ca}_{6}\left[\operatorname{Si}_{6}\operatorname{O}_{17}\right](\operatorname{OH})_{2} + 2\operatorname{Ca}(\operatorname{OH})_{2} = \operatorname{Ca}_{8}\left[\operatorname{Si}_{6}\operatorname{O}_{17}\right](\operatorname{OH})_{6}.$ Figures 1 and 2 show a structural scheme of foshagite and a frontal projection; figure 3 shows a plan in "Pauling's" (paulingovskiye) cylinders. It is easy to build a model of

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Crystalling Structure of Foshagite Ca₈[Si₅O₁₇](OH)₆

30**V/20-121-5-37/50**

of foshagite entirely of wollastonite chains (Fig 4), i.e. strictly according to formula

 $2\{400.3510_2.H_20\} = Ca_8[51_30_9]_2(OH)_4.$

Then the reaction taking place at 750° remains quite unintelligible, so far as a simple separation of water from the Ca-minerals (Ref 5) does not require any temperatures above 500°.

There are 4 figures and 11 references, 6 of which are Soviet.

ASSOCIATION:

Institut khimii Akademii nauk AzerbSSR (Institute of Chemi-

stry, AS Azerbaydzhan-SSR)

Institut kristallografii Akademii nauk SSSR (Institute of

Crystallography, AS USSR)

SUBMITTED:

May 7, 1958

Card 3/3

SOV/20-122-3-42/57

AUTHORS:

Simonov, V. I., Belov, N. V., Member, 4cademy of Sciences, 19002

TITLE:

The Crystal Structure of Seidhozerite (Kristallicheskaya

struktura seydozerita)

PERIODICAL:

Doklady Akademii nauk SSSR, 1958, Vol 122, Nr 3, pp 473-476

(USSR)

ABSTRACT:

On the basis of an analysis M. Ye. Kazakova gave the formula Na₂(Mn_{0,50}, Ti_{0,75}, Zr_{0,75})Si₂O₈(F,OH) for zirccnium titanium silicate (23% Zro₂, 13% Tio₂) found by Ye. I. Semenov called and downerite. According to optical and roentgen goniometry the

seidhozerite. According to optical and roentgen goniometry the mineral is monoclinic and has the cell parameters $a=5,\bar{5}3$, b=7,10, c=18,30 Å, and $\beta-102^{\circ}43^{\circ}$. The allegation that seidhozerite is holohedral was confirmed by the amplitude statistics $/F_{h01}/$; by means of this statistics a clear (accord-

ing to Ref 2) centrosymmetric distribution could be observed. According to the specific weight d = 3,47 the problem arose as to the realization of the structure with 3 Ti- and 3 Zr-atoms per cell in the P2/c group in which only 2- and 4-fold positions

Card 1/3

The Crystal Structure of Seidhozerite

SOV/20-122-3-42/57

are possible. It was not possible to draw reliable conclusions on the structure by means of the superposition method. The main results were obtained from the projection p(x,z). A regularity in the position of the peaks could be observed from this projection which was recently found by the authors for amblygonite (Ref 4). It once played an important part in the determination of the epidote structure (Ref 5). In seidhozerite 2 atoms with approximately equal atomic numbers must be placed in centers of symmetry translationally not identical which are at a distance of a/2 from each other. A further analysis of projection under consideration of the regularities of the syntheses of Paterson (given in Ref 6) mais possible the observation of two other heavy atoms. The relative position of the 4 atoms observed was used for the superposition of the Paterson projection and for the construction of $M_6(x,z)$. The latter furnished the first surface model of the structure. This was lateron determined more

surface model of the structure. This was lateron determined more precisely by the computation of the signs and by the computation of the projections $\sigma(x,z)$. After having returned to projection (y,z) the authors determined the sign of $F_{\text{Ok}\,1}$ by means of the direct (statistic) method (Refs 7.8). Then $\sigma(y,z)$ was construct-

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The Crystal Structure of Seidhozerite

SOV/20-122-3-42/57

ed. A precise projection $\sigma(x,z)$ made possible the determination of the grain ratio from $\sigma(y,z)$, and the determination of the latter by means of the normal method. The assumed coordinates of the 17 base atoms (43 parameters) are given on table 1. Seidhozerite proved to be a diorthosilicate inspite of its orthosilicate empirical molecular formula. The 8th 0-atom contained in the chemical formula is not a component of the silicon oxygen radical. The crystallochemical formula of seidhozerite must be set up as follows: Na₄MnTi($Zr_{1,5}$, Ti_{0,5})0₂(F,OH)Si0₇2. There are 2 figures, 1 table, and 11 references, 9 of which are Soviet.

SUBMITTED:

July 31, 1958

Card 3/3

3(8) Mamedov, Kh. S., Belov, N. V., AUTHÒRS:

SOV/20-123-1-44/56

Member, Academy of Sciences, USSR

TITLE:

The Crystal Structure of Tobermorite (Tobermorites) (0 kristallicheskoy strukture tobermorita (tobermoritov))

PERIODICAL:

Doklady Akademii nauk SSSR, 1958, Vol 123, Nr 1, pp 163 -

165 (USSR)

ABSTRACT:

Tobermorites are fibrous and at the same time platy, micalike Ca-hydrosilicates. They take on considerable amounts of water in the same manner as montmorillonite and vermiculite, remaining monocrystalline. There is only a corresponding enlargement of the parameter of the elementary cell. The water content in tobermorites increases in sharp, jump-like increments, a characteristic which distinguishes them from the above-mentioned clay minerals. Each increment has been given a different name. All tobermorites are characterized by rhombic symmetry (Ref 1). Their constants and properties are described. If the various amounts of inter-layer water are left out of consideration, the composition of all tobermorites is the same. One "tobermorite from Lokh-Eynort" (Ref 2) differs from all others. Its parameter corresponds

Card 1/4

The Crystal Structure of Tobermorite (Tobermorites) SOV/20-123-1-44/56

form-wise to an 11 A hydrate: it changes into criented fibers of wollastonite, but its basic cleavage is not (001) but (100)-like and it cannot be changed to a 14 A hydrate even after being ground to a fine powder and treated with water for many hours. Megaw and Kelsey (Ref 3) presented a structure scheme which agrees satisfactorily with the dif-fraction picture of an 11 A hydrate. They work from the assumption that of most importance are the wollastonite chains, (Sio 300, which are characteristic of the product of their thermal reactions. The chains are responsible for the fiberlike form of the tobermorite: the sheet-like structure is a result of condensation of the amphibole chains to talc nets. The silicon-oxygen nets are (according to Ref 3) similar to corregated cardboard. The authors develop the concrete structure of tobermorite sheets from these schemes. The authors' recent deciphering of the experiment which yielded okenite (Ref 6) among other things (Ref 7) shows that if the disintegration products of Ca-hydrosilicates at ~750° are wollastonite fibers with simple chains, (Si30c).

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The Crystal Structure of Tobermorite (Tobermorites) SOV/20-123-1-44/56

=3(SiO_x) then the double silicon-oxygen chains from xonotlite, (Si₆0₁₇ % (Ref 8) serve to generate in the hydrothermal syntheses of Ca-silicates. These chains are discrete in xonotlite itself. In okenite the double chains are no longer discrete and intertwine in a parallel manner, but about a half period of displaced, that is, displaced along the chain axis. Okenite nets are entirely flat in talc and also in mica. In tobermorite the okenite bonds are shoved over each other on swelling (Fig 1). Figure 1 shows an approximate localization of the Si-tetrahedra, 12 of which occur in every sheet (4 overlapping and 4 single pairs) and of the 20 cations of Ca (10 overlapping pairs); all 12 hydroxle groups, OH, (per whole cell) occur under non-covering O atoms in the horizontal bonds of the xonotlite rings. The position of the 16 (per cell) inter-layer H₂O is more difficult to determine. The paradox of the Lokh-Eynort tobermorite is satisfactorily eliminated if the electronogram (of Ref 2) is studied. The period here clearly shown is not 2.5.5 = 11 Å, as in normal tobermorites, but 3.5.5 = 16.5 Å. Thus the parameters a and

Oard 3/4

The Crystal Structure of Tobermorite (Tobermorites) SOV/20-123-1-44/56

b of the Lokh-Eynort tobermorite are proven to be a repetition of the xonotlite parameter with a c parameter which amounts to three-fold. There are 2 figures and 9 references, 3 of

which are Soviet.

ASSOCIATION: Institut khimii Akademii nauk AzerbSSR (Institute of Chemistry,

Academy of Sciences, Azerbaydzhanskaya SSR)

Institut kristallografii Akademii nauk SSSR (Crystallography

Institute, AS USSR)

SUBMITTED: August 1, 1958

Card 4/4

SOV/20-123-4-47/53 3(8) Mamedov, Kh.S., Belov, N. V. AUTHORS: Academician The Crystal Structure of Hillebrandite (O kristallicheskoy TITLE: strukture gillebrandita) Doklady Akademii nauk SSSR, 1958, Vol 123, Nr 4, pp 741-743 PERIODICAL: (USSR) A considerable number of calcium silicates invert to fibrous β -wollastonite (CaSiO $_3$) at 700-800 $^{\circ}$. These fibers are ABSTRACT: oriented parallel to the b axis (b=2. 3.65 %) which is common to the wollastonite and original silicate. From the authors' works (Refs 1-3) it is seen that wollastonite chains (3/SiO₃/₂ = /Si₃O₉/₂ are not the primary structural blocks in hydrothermal synthesis (either natural or artificial) of calcium (hydro)-silicates. These blocks are much more complex chains which originate by doubling of the wollastonite chains (/Si₆0₁₇/10-). These latter have been designated xonotlite chains (Ref 1). In the calcium (hydro)-silicate minerals they are present either unchanged (Refs 2,3) or condense to lattices (Refs 2,4). Hillebrandite is a characteristic and Card 1/3

The Crystal Structure of Hillebrandite

SOV/20-123-4-47/53

predominant product produced by hydrothermal synthesis through temperature decrease (pot sediment) (Ref 6). It precipitates easily with a surplus of Ca(OH)2 and even builds an oriented intergrowth with the latter. It is an arcicular and at the same time platy mineral. However, hillebrandite distinguishes itself markedly from okenite and tobermorite, primarily because it cannot be changed to oriented wollastonite through thermal treatment (Ref 5). Two of the 3 cell parameters agree exactly with those of xonotlite (Ref 5). This paradox - that is the undoubted role of xonotlite in the wollastonite reaction and the non-inversion of hillebrandite to wollastonite by thermal treatment - can easily be explained if 2 subtractions are made. If (a) the basic molecule of xonotlite is removed from the formula of hillebrandite and (b) the 2 unequal parameters, c, are subtracted, the results show that the hillebrandite cell is made of alternating layers of xonotlite and portlandite (Fig 1). cannot be taken literally, however, for hillebrandite when compared with zonotlite has the following characteristics: the central sheet with 2 chains, /Si6017/4, contains its "own"

Card 2/3

The Crystal Structure of Hillebrandite

SOV/20-123-4-47/53

calcium-cation layer both above and below, while in xonotlite the calcium-cation layer always belongs to both central layers of /Si6017/c chains. From this scheme it can be seen that the perfect cleavage (001) runs through the middle of the portlandite layer which has become a constituent part of the hillebrandite. There are 1 figure and 6 references, 5 of

ASSOCIATION:

Institut khimii Akademii nauk AzerbSSR (Chemistry Institute of the Academy of Sciences of the Azerbaydzhanskaya SSR) Institut kristallografii Akademii nauk SSSR (Crystallography Institute, Academy of Sciences, USSR)

SUBMITTED:

August 1, 1958

Card 3/3

BELOV, N.V.

Studies on structural mineralogy. Part 9. Min.sbor. no.12: 15-42 '58. (MIRA 13:2)

1. Institut kristallografii AN SSSR. (Crystallography)

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isezoyuznoye sovesuzhaniye po stekloobrannoru sostoyaniyu. 3d, Leningrad, 1959.

Stekloobrarnoys scatoganiys; trudy Tret 'yego vestoyuznogo sowsthchaniya Laningrad, 16-20 noyabrya 1959 (Vitrecus State; Transactions of the Third All-Union Conference on the Vitrecus State, Held in Laningrad onlowederif-20, 1959) Wascoy, Isd-ro AN ESSS, 1960, 54 p. Errata allp inserted. 5,200 copies printed. (Series: Its: Trudy)

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APPROVED FOR RELEASE: 06/06/2000

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| | Vitreous State (Cont.) | ě. | Yevstrop'yev, K.S. | Demkins, L.I. J | Berborodov, K. | | Myuller, R.L. Glass-Forsing | Sorrmova, K.A. | Tarasov, V.V. | Card 6/22 | • | Vitreous | | Belov, H. | Discussion | | Avgustinik, A.I. | | Mel'nichenko, L.(| Lepinski) Conducti | | Vitreous State | Yernolcako, N.N. | Chechilin | Sryvalin, of Call-Fe | Discussion | | Yol'kensh Yitreous | Anufriyev | Bolotina, I.A. Card 8/22 | • |
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Belov, N.V.

"The Second Chapter of the Crystall Chemistry of Silicates"

Areport presented at Symposium of the International Union of Crystallography
Lenningrad 21-27 May 1959

SO: B 3,135, 471 28 July 1959

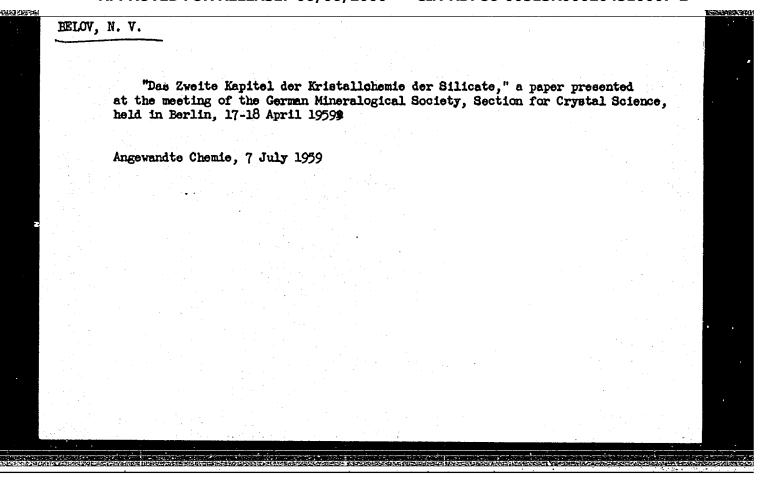
NIKOLAY VASILYEVICH BELOV; GEORGIY BORDSOVICH BOKIY; ILLARION ILLARIONOVICH SHAFRANOVSKIY

"IN MEMORIUM OF E.S. DFEDOROV"

A Report presented at Symposium of the International Union of Crystallography Lenningrad, 21-27 May 1959

SO; B, 3135, 471

28 July 1959



3(8) AUTHOR:

Belov, N. V.

SOV/7-59-3-11/13

TITLE:

Concerning Paper by A. A. Beus "On the Position of Alkali Metals in the Structure of Beryl" (Po povodu raboty A. A. Beusa "O polozhenii shchelochnykh metallov v strukture berilla")

PERIODICAL:

Geokhimiya, 1959, Nr 3, pp 282-283 (USSR)

ABSTRACT:

The author considers it to be unjustified to tear the aluminum portion of beryl apart, especially because the five analyses mentioned by A. A. Beus give nearly exactly two atoms Al per formula unit of beryl. It is much more probable that here lithium replaces beryllium. This is indicated by the nuclear-chemical affinity between lithium and beryllium. Besides, the ion radius of lithium, according to Pauling, amounts to only 0.60 A as against the value of 0.78 A according to Goldschmidt, and that value increases still more in the case of a covalent bond in fourth coordination. In any case, it is not permissible to declare that any isomorphism exists between beryl and milarite and herefrom to draw conclusions concerning beryl structure. There is 1 Soviet reference.

Card 1/2

AUTHORS: Simonov, V.I. and Belov, N.V. SOV/70-4-2-4/36

TITLE: The Determination of the Crystal Structure of goldozerite

(Opredeleniye struktury seydozerita)

PERIODICAL: Kristallografiya, 1959, Vol 4, Nr 2, pp 163-175 (USSR)

ABSTRACT: Seydozerite from the Seydozero area has the formula Na2 (Mn0.5 Ti 0.75 Zr 0.75) Si 2 08 (F,OH) as described in the

work of Semenov, Kazakova and the author (Ref 1). It is

monoclinic with the space group

 $C_s^2 = Pc$ or $C_{2h}^4 = P2/c$ and the cell dimensions

 $a = 5.53 \pm 0.2 \text{ Å}$ [sic] $b = 7.10 \pm 0.03 \text{ Å}$,

 $c = 18.30 \pm 0.10 \text{ Å}$ and $\beta = 102^{0}43' \pm 1'$. β was

found by optical goniometry. Possible centro-symmetry is indicated by the morphology, twithe *baence of piezo-electricity and by the statistics of the hol intensities. The Patterson functions (projections) confirmed this and the holohedric group P2/c was assumed.

 $d_{obs} = 3.47$ gives $Z = 3.87 \simeq 4$ formulae units per cell.

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SOV/70.4-2-4/36 The Determination of the Crystal Structure of Seydozerite

378 non-zero reflexions in the hol zone and 331 in the okl zone were used in the analysis. The absorption for $\lambda = 0.71$ Å was 35 cm⁻¹ and the cross-sections of the crystals used were 0.15 x 0.20 mm (hol) and 0.3 x 0.5 mm okl. This leads to errors in |F| of up to 10% and 15%, respectively. P(y,z) and P(x,z) were calculated and are reproduced. The heavy Zr-Zr peaks could be identified and used for superposition methods in the (x,z) projection. Statistical sign-determination methods were found very suitable for the F(okl) reflexions as the space group P2/c is appropriate. For these reflexions those with l = 2n have:

F(okl) = F(okl) = F(okl) = F(okl) and those with l = 2n + 1 have F(okl) = -F(okl) = -F(okl) = F(okl).

70 reflexions with the greatest unitary structure amplitudes were taken as "bankers". The signs were considered found if \searrow 3 pairs gave the same sign.

264 out of 331 signs were thus allotted. The Fourier projection was then calculated. It showed a systematic,

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The Determination of the Crystal Structure of Seydozerite

over-regular atomic arrangement which made superposition methods invalid and caused the statistical method to give ~ 25% of incorrect signs. Crystallochemical and mineralogical considerations concerning the isomorpous replacement had to be used in assigning the atomic positions (see Table 1, p 168). The accuracy of the atomic positions estimated by Vaynshteyn's method was $Zr \pm 0.001$, Mn ± 0.002 ; Ti ± 0.003 ; Si ± 0.004 :
Na ± 0.005 ; O ± 0.009 Å . All x-coordinates come from $\rho(x,z)$ where there are no non-overlapping maxima. were calculated from the coordinates and hol and Fokl compared with the experimental values, giving reliability factors of 17.2 and 22.5% for hol and okl, reflexions $(F_{exp} \neq 0 \text{ up to sin } \frac{1}{30})$ and $F_{exp} \neq 0$ up to sin \$/λ <0.66), respectively. Without counting F reflexions, the values were 16.6 and 20.7%. Counting up the bond strength balance according to Pauling's second rule, there are some deviations of 25%.

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The Determination of the Crystal Structure of Seydozerite

The formula can be written structurally as $\operatorname{Na_{h}MnTi}(Zr_{1.5}\operatorname{Ti}_{0.5})_{0.2}(F,0H)_{2}[\operatorname{Fi}_{2}0_{7}]_{2}$ with E=2. There are endless sheets of octahedra threaded on the twofold azis. Atoms of $\operatorname{Mn}(\operatorname{Mg})$, Ti and Na alternate in these octahedra. Zr and Na octahedra alternate in double bands along the b-axis. The silicate groups are $\operatorname{Si}_{2}0_{7}$ double tetrahedra parallel to b. Cuspidine and tilleyite have similar bonds between diorthogroups and Ca-octahedra. The bond distances are tabulated and analysed. The OOl cleavage is parallel to the sheets of octahedra. Optical measurements gave $2V=+68^{\circ}$. of octahedra. Optical measurements gave $2V=+68^{\circ}$. with a and n_{p} with b and this is consistent with the structure, the Mn octahedra accounting for most of the refractivity.

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The Determination of the Crystal Structure of Seydozerite

There are 6 figures, 3 tables and 21 references, 15 of which are Soviet, 2 international, 3 English and 1 German

ASSOCIATION: Institut kristallografii AN SSSR (Institute of Crystallography of the Ac.Sc.USSR)

SUBMITTED: January 21, 1959

Card 5/5

AUTHOR: Below, N. W. SOV/70-4-2-36/36

TITLE: The Hexagonal Space Groups (Geksagonal'nyye

fedorovskiye gruppy)

PERIODICAL: Kristallografiya, 1959, Vol 4, Nr 2, pp 268 - 276 (USSR)

ABSTRACT: Didactic article on the properties of the space groups.

There are 12 figures and 3 references, 2 of which are

Soviet and 1 German.

ASSOCIATION: Institut kristallografii AN SSSR

(Institute of Crystallography of the Ac.Sc.USSR)

SUBMITTED: December 1, 1958

Card 1/1

sov/70-4-3-3/32

Belov, N.V. and Klevtsova, R.F. AUTHORS:

The Simplest Method of Deducing the Fedorov (Space)

TITLE:

PERIODICAL: Kristallografiya, 1959, Vol 4, Nr 3, pp 289-292 (USSR)

For pedagogic purposes it is most convenient to start with the clases mm2 and mmm and primitive lattices. ABSTRACT:

The symmetry elements m, n, c, g(= a or b) are selected three at a time with the limitation that they do not change from one to another by the simple intercharge of axes. The method rests on the principle that, if all the symmetry elements of a space group are moved so that they intersect in a point and glide and screw translations are suppressed, the appropriate point group is obtained. In expanding from a point group centres of

symmetry (i) are generated from i by, for example, $i_{1/2\ 00} = i \times a$, $i_{0\ 1/2\ 1/2} = i_{000} \times (b + c)$,

 $\frac{1}{1/2} \frac{1}{2} \frac{1}{2} = \frac{1}{000} \times (a + b + c)$. The displacements of m planes can be found by the operational equation

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The Simplest Method of Deducing the Fedorov (Space) Groups

$$_{o^{m}x} \times a/2 = _{1/4}^{m} \times .$$

There are 16 primitive groups corresponding to Pmmm. These are given by adding translations to the m planes as:

$$Pm + 0, m + 0, m + 0 = Pmmm;$$

$$Pm + 0$$
, $m + a/2$, $m + a/2 = Pmaa$;

$$Pm + a/2, m + 0, m + a/2 = Pm^{x}ma$$

where the asterisk denotes a displacement of the plane from the origin (from the original centre of symmetry). The other groups are given, for example:

$$Pm + b + c$$
, $m + c + a$, $m + a + b = Pnnn$

$$Pm + a + b$$
, $m + b + c$, $m + c + a = Pb^{M}c^{M}a^{M}$

Similarly, 10 primitive groups can be derived from the

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sov/70-4-3-3/32

The Simplest Method of Deducing the Federov (Space) Groups

class min2 , for example:

$$D_2^1 = P 222; \quad D_2^2 = P 2, 2 + c, 2 + c = P22^{2}2;$$

$$D_2^3 = P^2 + a + b, 2 + b + a, 2 + 0 = P_1^{x_2} = P_1^{x_2}$$

$$D_2^4 = P2 + a + b, 2 + b + c, 2 + c + a = P2_1^{k_2} 2_1^{k_2}$$

This method of deducing the space groups is closer to Fedorov's original method than to Schoenflies' (Ref 5). There are 6 references, of which 3 are Soviet, 2 German and 1 international.

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sov/70-4-3-3/32 The Simplest Method of Deducing the Fedorov (Space) Groups

ASSOCIATION: Institut kristallografii AN SSSR (Institute of

Crystallography of the Ac.Sc., USSR)

SUBMITTED: April 13, 1959

Card 4/4

Pavlov, P.V. and Belov, N.V. Sov/70-4-3-8/32 · AUTHORS:

The Determination of the Structures of Herderite, Datolite TITLE:

and Gadolinite by Direct Methods

FERIODICAL: Kristallografiya, 1959, Vol 4, Nr 5, pp 324 - 340 (USSR)

ABSTRACT: The structures of these three compounds were determined in parallel by direct methods, particularly by those elaborated in the Institute of Crystallography and in Gor'kiy University, which proved to be exceptionally powerful. A full account is given for pedagogic purposes. The cell dimensions and space group, found by Strunz, for herderite 5(a = 9.80, b = 7.68, c = 4.80 Å, $\beta = 90^{\circ}06^{\circ}$, $C_{2h}^{\circ} = P2_{1}/a$) were confirmed. dobs. and Z = 4, the formula unit being CaBePO_LF. The use of Harker-Kasper inequalities followed by Zachariasen's statistical analysis has been successful several times

before and was applied here. Weissenberg photographs with Mo radiation provided abundant data. There were 167 independent hkO reflexions. Amplitudes were put on an absolute scale by Wilson and Vaynshteyn's methods.

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The Determination of the Structures of Herderite, Datolite and Gadolinite by Direct Methods

There were 15 with $\left| U_{hk0} \right| > 0.5$. In all, 45 confirmed sign relationships of the form $S_{H+K} = S_H \cdot S_K$ were found. 18 signs were found uniquely by:

$$\left| {^{U}}_{hk} \right|^{2} \leqslant 1/2 + 1/2 \, U_{2h, 2k, 2l}$$

and other inequalities and less directly others giving a total of 56 "banker" reflexions. Two signs were given arbitrarily. Zachariasen's method was then applied and gave another 84 signs, i.e. a total of 140 out of 167. $^{\circ}$ 70% . About 20-24 pairs determined each sign. The resulting Fourier projection showed all atoms and calculated those gave R=24% only two having signs opposite to those assumed. A second synthesis with the remaining 27 reflexions and recalculation with the new positions gave R=14.9% without zeros and 20.4% with zeros up to sin $\theta/\lambda=1.1$. Normalisation by $\sum_{c} F_{c}$ showed that the

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The Determination of the Structures SOV/70-4-3-8/32 Gadolinite by Direct Methods

original setting of the amplitudes on an absolute scale was accurate to within 5%. The hol projection was treated similarly. There were 116 non-zero reflexions, Uhol > 0.5 . Without zeros R = 14.3% and with 60 zeros up to 1.1 R = 19.7% . Vaynshteyn's method gave the probable errors in atomic positions as follows: for Ca 0.004 A; Po-0.006 A; Be - 0.033 A; O-0.015 A and F-0.013 A. Table 1 gives the atomic co-ordinates in the structures of herderite, datolite and gadolinite (in hundredths of a, b and c). Datolite I represents Japanese data and datolite II Pavlov and The structure consists of infinite pseudotetragonal nets of PO4 and BeO3F tetrahedra. In the net the fourfold centrosymmetrical rings of tetrahedra of two sorts alternate with locked centrosymmetrical pulled-out octagons of the same tetrahedra. This is characteristic of felspars and other related aluminosilicates. The

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The Determination of the Structures of Herderite, Datolite and Gadolinite by Direct Methods

structure has two storeys, the lower consisting of 4 antiprisms (with 8 corners) around the Ca atoms and the upper of linked PO_{4} tetrahedra in one orientation and BeO_{5} F tetrahedra in another. Interatomic distances are tabulated. Pauling's valency balance does not fit very accurately for some 0 atoms. CaBSiO₄(OH), datolite (a = 9.62, b = 7.60, c = 4.84 Å, $\beta = 90^{\circ}$, $P2_{1}/a$) was solved by Ito and Mori by a semiheavy atom technique. The analysis reported for herderite was repeated. It was also partially repeated for gadolinite, $Fe^{++}Y_{2}Be_{2}O_{2}Si_{2}O_{8}$ (Z = 2, a = 9.89, b = 7.52, c = 4.71, $\beta = 90^{\circ}$ 53') with results given in the table. Fe atoms are found at the origins octahedrally co-ordinated but otherwise the structure is very similar to that of the other minerals.

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"APPROVED FOR RELEASE: 06/06/2000 CIA-RDP86-00513R000204510007-2

The Determination of the Structures of Herderite, Datolite and Gadolinite by Direct Methods

There are 8 figures, 7 tables and 19 references, 13 of which are Soviet, 2 German and 4 international.

ASSOCIATION: Institut kristallografii AN SSSR (Institute of Gor'kovskiy universitet im. N.I. Lobachevskogo (Gor'kiy University imeni N.I. Lobachevskiy)

SUEMITTED: February 23, 1959

Card 5/5

. AUTHORS:

Belov, N.V. and Klevtsova, R.F. sov/70-4-4-3/34

TITLE:

Moreconnect the Simplest Way of Developing the Fedorov

PERIODICAL: ABSTRACT:

Kristallografiya, 1959, Vol 4, Nr 4, pp 473-476 (USSR) The development of the 230 space groups by the methods outlined in Kristallografiya, 1959, Vol 4, Nr 3, still presents some difficulties in dividing the translations

introduced by various symmetrical and semi-symmetrical means. Even without a diagram it is possible to allocate a star, denoting displacement from the origin, to the planes in the space group symbol (in the first instance for the orthorhombic system). This is best done by writing down each halving. For example, Pbcn is

expanded as Pm+b, m+c, m+a+b and should be written Pbxcnx . All 16 primitive orthrohombic groups based

on Pmmm are listed. The method is particularly suitable also for obtaining the tetragonal groups in the standard form. The remainder of the paper is devoted to showing

Card1/2

More on the Simplest Way of Developing the Fedorov (Space) Groups how these can be obtained. Various modifications of the for the special point on the inversion axis 7 is used There are 4 figures and 4 references, 3 of which are Soviet and 1 English.

ASSOCIATION: Institut kristallografii AN SSSR (Institute of SUBMITTED: May 15, 1959

Card 2/2

AUTHOR: Belov, N.V.

sov/70-4-4-26/34

fitle:

On Covariant and Contravariant Relationships Between Derivative and Generating Structures

PERIODICAL:

Kristallografiya, 1959, Vol 4, Nr 4, pp 618-619 (USSR) ABSTRACT: Transformations of covariant coordinates (indices) and contravariant coordinates (axial indices, points) are always given in textbooks but it is not always clear Whether this relates to transformations of coordinates for a change of axes in the same structure and in the same lattice. This is not so: the corresponding formulae and tables are most convenient when the structure has some simple motive which does not describe all details of the structure but where the crystal cell is larger and more complicated than the cell of the pure motive. This is illustrated with clinohumite MgF2.4Mg2SiO4 where the unit cell contains 9 of the Si-O sheet motive units

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On Covariant and Contravariant Relationships Between Derivative and Generating Structures

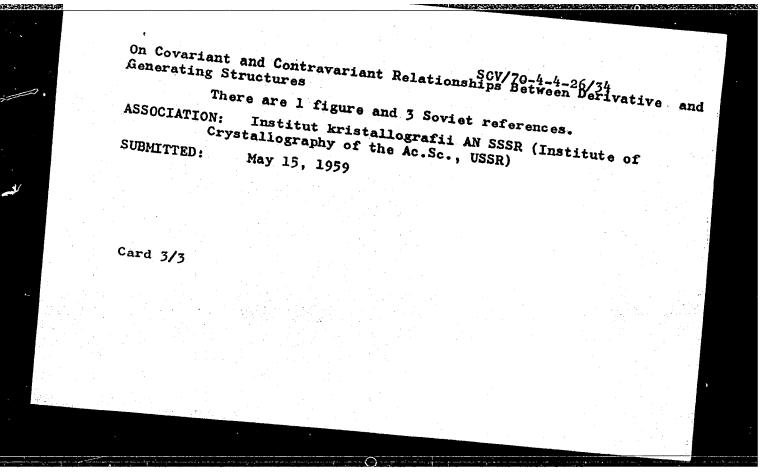
$$A = \frac{9}{2}a - c$$
, $a = \frac{2}{9}A + \frac{2}{9}C$

where large letters apply to the full cell and small letters to the motive unit. The coordinates transform:

$$X = \frac{2}{9} x \qquad Z = Z + \frac{2}{9} x$$

Hence, for Mg at the centres of octahedra, we get, from 1.0, 2/9, 2/9; from 2.0, 4/9, 4/9; from +1/2, -1/2-1/9, -7/18. For Si at the centre of the triangle between octahedra with coordinates 3/2, 1/6, we get 1/3, 1/2, etc.

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24.710

76003

AUTHOR:

Belov, N. V.

SOV/70-4-5-25/36

TITLE:

On the Nomenclature of the 80 Plane Groups in Three Dimensions

PERIODICAL:

Kristallografiya, 1959, Vol 4, Nr 5, pp 775-778 (USSR)

ABSTRACT:

Reviewing the historical aspects of symbolizing these groups, the author rejects W. T. Holser's inaccurate statements (Z. Kristallogr., 110, 266, 1958) and criticizes W. Cochran's application of international symbols two-sided plane groups. Advancing his own earlier in 5 different symbols, some of the 80 plane groups A. V. Shubnikov's principle of colored symmetry. The described by three different symbols. There is 1 lefterences, 4 Soviet, 4 German, 2 Danish,

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"APPROVED FOR RELEASE: 06/06/2000 CIA-RDP86-00513R000204510007-2

On the Nomenclature of the 80 Plane Groups in Three Dimensions

ASSOCIATION:

76003 SOV/70-4-5-25/36

Crystallographical Institute of the Academy of Sciences of the USSR (Institut kristallografii AN SSSR)

SUBMITTED:

August 13, 1959

Card 2/2

0.0000

76012

SOV/70-4-5-34/36

AUTHORS:

Belov, N. V., Vaynshteyn, B. K., Kitaygorodskiy, A. I., Poray-Koshite, M. A., Semiletov, S. A., Sheftal', N. N.

TITLE:

International Fedorov Session on Crystallography Held in

Leningrad

PERIODICAL:

Kristallografiya, 1959, Vol 4, Nr 5, pp 796-800 (USSR)

ABSTRACT:

The International Union of Crystallography (IUC) and the Academy of Sciences of the USSR convened an International Session (interim) on Crystallography commemorating the 40th anniversary of the death of the great Russian crystallographer Ye. S. Fedorov. The session, attended by 600 scientists from the USSR, U.K., France, U.S., Japan, Germany, Czechoslovakia, Netherlands, Canada, Australia, and other countries, was held in Leningrad from May 21 to 27, 1959. The major reports were presented to the plenary sessions and some 100 reports to 2 panels. subject of the 1st panel was crystal-chemical analysis and that of the 2nd panel electron was diffraction studies.

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International Fedorov Session on Crystallography Held in Leningrad

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The reports to the plenary sessions were presented by the following Soviet scientists: N. V. Belov (VP of IUC), W. I. Simonov, V. A. Frank-Kamenetskiy, G. B. Bokiy, M. A. Poray-Koshits, L. O. Atovmyan, G. N. Tishchenko, A. B. Ablov, T. I. Malinovskiy, Ye. A. Shugam, V. M. Levina, Yu. S. Terminasov, Sh. Kh. Yar-Mukhamedov, Ya. S. Umanskiy, V.I. Iveronova, L. S. Palatnik, V.A. Finkel', Sonin, I. S. Zheludev, I. G. Ismailzade, I. S. Rez, Sonin, I. S. Zheludev, I. G. Ismailzade, I. S. Rez, Z. V. Zvonkova, A. I. Kitaygorodskiy, O. V. Stavrovskiy, N. N. Sandakova, N. M. Bashkirov, B. K. Vaynshteyn, I. M. Trifonov, B. M. Shchedrin, D. M. Kheyker, M. M. Uman-The reports of the U.S. crystallographers were presented J. Donohue, G. Donnay, J. H. D. Donnay, and W. Parrish. Six reports were presented by British crystallographers, 2 by German, 2 by Czech, 2 by Dutch and 1 each by

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International Fedorov Session on Crystallography Held in Leningrad

76012 SOV/70-4-5-34/36

French, Canadian, and Japanese crystallographers. The session admitted five new member nations into IUC, confirmed its newly appointed officers, including the editor of "Acta Crystallographica," A. J. C. Wilson, appointed G. B. Bokiy as head of the subcommittee for abstracting the Soviet publications in crystallography, planned Japan to be the site of the next interim, and Italy or Israel of the next congress, and solved some other business matters.

SUBMITTED:

July 1, 1959

Card 3/3

24.7100

77100 SOV/70-4-6-1/31

AUTHORS:

Neronova, N. N., Belov, N. V.

TITLE:

Ferromagnetic and Ferroelectric Space Groups

PERIODICAL:

Kristallografiya, 1959, Vol 4, Nr 6, pp 807-812 (USSR)

ABSTRACT:

The authors selected 31 ferroelectric point groups out of 90 point groups of the Shubnikov classification (plus-minus groups, groups of antisymmetry, black and white groups) in a similar way as they previously had selected 31 ferromagnetic point groups out of the same 90 point groups. The principal differences between the ferromagnetic and ferroelectric groups are: (1) the former's symmetries are subdivisions of the limiting axial vector symmetry described by

 $\frac{\infty}{m} \frac{2^{\prime}}{m^{\prime}} \frac{2^{\prime}}{m^{\prime}}$, and of the latter's by $\frac{\infty}{m^{\prime}} \frac{2^{\prime}}{m} \frac{2^{\prime}}{m}$; superscripts

denote antisymmetry elements, (2) ferroelectrics require absence of a center of symmetry, 1, while

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Ferromagnetic and Ferroelectric Space Groups

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ferromagnetics require a center of antisymmetry, 1', (3) equator planes are mirrors in ferromagnetic groups and colored (black and white) planes in ferroelectrics, (4) longitudinal planes, on the contrary, are mirrors in ferroelectric groups and colored planes in ferromagnetic groups. The symbolic descriptions of 10 axial groups out of 31 are outwardly identical in both cases but ferromagnetism and ferroelectricity never occur in the same group because of internal "micro" discrepancy. The same is true in the case of 2'mm' point group of which ferroelectric and ferromagnetic space groups differ from one another because of relocation of two different planes. On the basis of these distinctions, 275 ferromagnetic and 275 ferroelectric space groups are selected out of the 1651 space groups of the Shubnikov classification and compiled in a four page table that describes the included point and space groups in international symbols. There is I table; and 6 references, 5 Soviet, 1 Danish.

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"APPROVED FOR RELEASE: 06/06/2000 CIA-RDP86-00513R000204510007-2

Ferromagnetic and Ferroelectric

Space Groups

77100

SOV/70-4-6-1/31

ASSOCIATION:

Crystallographical Institute of the Academy of Sciences of the USSR (Institut kristallografii AN SSSR)

SUBMITTED:

September 1, 1959

Card 3/3

"APPROVED FOR RELEASE: 06/06/2000 CIA-RDP86-00513R000204510007-2

24.7100

†7118 SOV/70-4-6-19/31

AUTHOR:

Belov, N. V.

TITLE:

Concerning the Basic Theorem of Close-Packed Arrangement

of Globuli. Brief Communication

PERIODICAL:

Kristallografiya, 1959, Vol 4, Nr 6, pp 918-919 (USSR)

ABSTRACT:

Having stated that no textbook on crystal chemistry and crystal structures known to him, including the one written by himself, convincingly illustrates the fact that close-packed three-layer arrangement produces close-packed face-centered cubic structure, the author seeks to illustrate this by using ABC layers. Of these the A layer contains I globule or 7 globules, as in usual illustrations, but the B and C layers contain 6 globuli, instead of 3, forming triangles turned 180° relative to each other. Placing 7-globule A-layer between 6-globule B and C layers produces an octahedron with two horizontal faces. Placing 1-globule A layer between B and C, and the next A on C, produces a face-centered cube.

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"APPROVED FOR RELEASE: 06/06/2000 CIA-RDP86-00513R000204510007-2

Concerning the Basic Theorem of Close-Packed Arrangement of Globuli. Brief Communication

77118

SOV/70-4-6-19/31

No octahedron in close-packed structure can have a common face with an adjacent octahedron, but only with a tetrahedron. The latter is produced by placing a C layer on an octahedron face, a 1-globule A on C, and a B on A,

There are 5 figures; and 1 Soviet reference.

ASSOCIATION:

Crystallographical Institute of the Academy of Sciences of the USSR (Institut kristallografii AN SSSR)

SUBMITTED:

September 1, 1959

Card 2/2

D.P. Serdiuchenko's calciotalc. Zap. Vses. min. ob-va 88 no. 3:305-308
'59. (MIRA 12:11)

1. Deystvitel'nyy chlen Vsesoyusnogo mineralogicheskogo obshohestva.

(Talc)

3(8)

507/20-125-2-41/64

AUTHORS:

Belov, N. V., Academician

TITLE:

On the Crystalline Structure of Hurlbutite (O kristallicheskoy

strukture kherlbutita)

PERIODICAL:

Doklady Akademii nauk SSSR, 1959, Vol 125, Nr 2, pp 383-385

(USSR)

ABSTRACT:

The mineral mentioned in the title CaBe P208 is known since 1952 (Ref 1). On the basis of crystallographic and radio-

graphic investigations carried out by the discoverer the mineral

was ascribed to rhombic syngony, especially to the older holohedral class D2h = mmm. Its further constants are recalled.

In the following year a structural similarity between hurlbutite and dunburite (Ref 2) was found. It may be seen from the mentioned data that the lattice constants of both minerals and their physical characteristics are very closely related in general; in the case of hurlbutite, however, the parameter a is somewhat larger. According to this fact (less solid packing) all refraction indices are lower. Both minerals mostly differ by the Fedorov groups. The authors could not

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solve this problem by a comparison of the indicated lines of

On the Crystalline Structure of Hurlbutite

807/20-125-2-41/64

the Debyegrams. For the purpose of determining the crystalline structure of hurlbutite the authors investigated this mineral in detail by means of X-ray analysis. For this purpose they used samples from South Rhodesia (Harvard Collection of Professor K. Frondel' and Hurlbut = Kheribut). The completely transparent splinters of a structure as isometric as possible of about 0.3 - 0.5 mm were adjusted according to the Lausdiagrams on the basis of the Umanskiy-Kvitko method. The Laueclass of hurlbutite was not defined to be D2h = mmm, as had been expected, but to be $C_{2h} = 2/m$. This mineral therefore does not belong to the rhombic syngony but to the moneclinic one with an angle $\beta \approx 90^\circ$. The identity periods in the directions of the 3 double axes which were determined from the radiograms agree (within the experimental error limits) with the data given in reference 1. The mineral clearly belongs to the Fedorov group. C5 = P2₁/a with a center of symmetry which is beyond any doubt. Two further beryllium phosphates: beryllonite (Ref 5) and herderite (Refs 5, 7) belong to the same group. The fact that hurlbutite belongs to the afcresaid group seems quite natural if one considers the circumstance that all 3 minerals are found closely intergrown which is due to their

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On the Crystalline Structure of Hurlbutite

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metasomatic development (Ref 8). In conclusion it is referred to the luminescence of hurlbutite under the action of X-ray and cathode ray which is not mentioned in publications. It is light-bluish-green and remains so for 5-10 minutes after the cease of the irradiation. Its reason has not yet been explained. This may be an important diagnostic criterion. There are 8 references, 1 of which is Soviet.

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TITLE:

Isomorphous Interactions Between Zirconium and Titanium (Obizomorfnykh sootnosheniyakh mezhdu tsirkoniyem i titanom)

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ABSTRACT:

The present paper gives the correction by the authors who were not careful (Ref 1) in the case of several sentences: "Ti was constantly be found in all papers concerning the Lovozero masconstantly be found in all papers concerning the Lovozero masconstantly be found in all papers concerning the Lovozero masconstantly be found in all papers concerning the Lovozero masconstantly be found in Lovenite with a content of more than 20% ZrO₂ substituted up to 50% by TiO₂". There are, however, important reasons for the absence of Ti in the Zr-star. The present material from the Lovozero-massif shows that this isomorphism of Zr and Ti occurs in fact only in the case of three and Astrophyllite-Kupletskite. These minerals have a high manserite is quite clear (Refs 1,2) though this is not the case in the two last mentioned minerals (their structure is unknown).

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